

# XINXIN LIU

## Master's Student in Physical Chemistry

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## EDUCATION

### MSc in Physical Chemistry

MOE Key Laboratory of Theoretical Chemistry of Environment;  
School of Environment, South China Normal University

2022 – 2025

Guangzhou, China

CGPA: 3.99/5.00

### BSc in Applied Chemistry

College of Materials and Energy, South China Agricultural University

2018 – 2022

Guangzhou, China

CGPA: 3.93/5.00

## DISSERTATION WORK

### MSc Thesis

Analytical Electromagnetic Response Theory of HF/KS Energy: A  
Unified Treatment from Nonrelativistic to Relativistic Frameworks

- Reconstructed the analytical derivative theory for electromagnetic response properties within both HF and KS-DFT frameworks to avoid theoretical inconsistencies especially in dealing with dynamic electromagnetic response
- Revealed that the widely adopted GIAO method in calculating magnetic response properties cannot fundamentally eliminate the gauge dependence in time-varying fields
- Extended the new approach to relativistic two- and four-component frameworks and incorporated the case of non-collinear exchange-correlation functionals
- Developed a Python code for implementing the above methods in PySCF

### BSc Thesis

DFT Analysis of the Conversion Mechanism from Dihydroartemisinin  
Acid to Artemisinin

- Proposed a plausible reaction path
- Identified the initial dominant conformations using xTB
- Computed the thermochemical data using Gaussian
- Determined the rate-determining step of the reaction to optimize conditions for the drug production

## CERTIFICATES

- CET-6 Certificate
- NCRE-2 Certificate
- the **Second Price Award** in the Preliminary Round of the 2019 "FLTRP-ETIC Cup" English Writing Contest

## HOBBIES

**Exploring Nature and the World**  
Observing the nature of things

**Music Enthusiast**  
Enjoying quality music across various genres

**Reading and Lifelong Learning**  
Pursuing continuous learning and meaningful discussions

## LOOKING FOR

"To work in a progressive and dynamic research organization where one could solve scientific enigmas and contribute towards welfare of society"

## TECHNICAL STRENGTH

Fortran ● ● ● ● ●

C/C++ ● ● ● ● ●

Python ● ● ● ● ●

Bash ● ● ● ● ●

Tex ● ● ● ● ●

Git ● ● ● ● ●

MS Office ● ● ● ● ●

## MOST PROUD OF

**Top Performer in Master's Program**  
Achieved top position in the Diploma of Physical Chemistry program;  
Demonstrated a strong passion for natural sciences and a commitment to excellence in research

**Knowledge Evolution**  
Going next level everyday by perpetual learning of scientific and technical knowledge

## STRENGTHS

Thermodynamics & Statistical Mechanics

Linear Algebra

Quantum Chemistry

Theoretical & Computational Chemistry

Calculus

Classical Electrodynamics

Careful and Earnest

Hard-working

Flexible and Adaptable

## LANGUAGES

Chinese (Mandarin)

Cantonese

English

